

1,2,3-Trichloropropene
96-19-5 | DTXSID3047766

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.30×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 3.53×10^{-1}

Confidence level: 7.00×10^{-1}

Nearest Neighbors from the Training Set

Image not found

(Z)-Dichloropropene

Measured: 1.12×10^{-11}

Predicted: 1.42×10^{-11}

Image not found

trans-1,3-Dichloropropene

Measured: 1.12×10^{-11}

Predicted: 1.42×10^{-11}

Image not found

Dichloroacetaldehyde

Measured: 2.30×10^{-12}

Predicted: 2.47×10^{-12}

Image not found

Chloroacetaldehyde

Measured: 3.10×10^{-12}

Predicted: 4.01×10^{-12}

Image not found

Methylketene

Measured: 7.00×10^{-11}

Predicted: 6.39×10^{-11}

Image not found

Ethylketene

Measured: 1.18×10^{-10}

Predicted: 9.07×10^{-11}